Full wwPDB X-ray Structure Validation Report ⓘ

Jan 3, 2024 – 05:39 pm GMT

PDB ID	:	5LLY
Title	:	Photosensory Module of Bacteriophytochrome linked Diguanylyl Cyclase from Idiomarina species A28L
Authors	:	Gourinchas, G.; Winkler, A.
Deposited on	:	2016-07-28
Resolution	:	2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

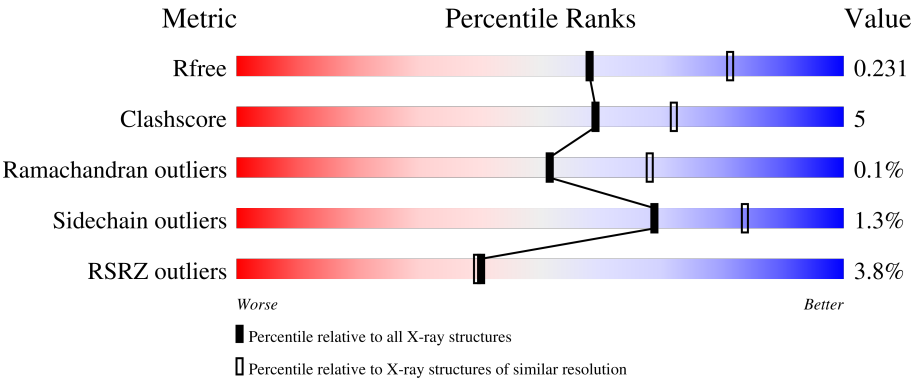
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	529	2% 85% 12% ·
1	B	529	7% 79% 13% 7%
1	C	529	4% 84% 12% ·
1	D	529	% 81% 14% 5%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 16833 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

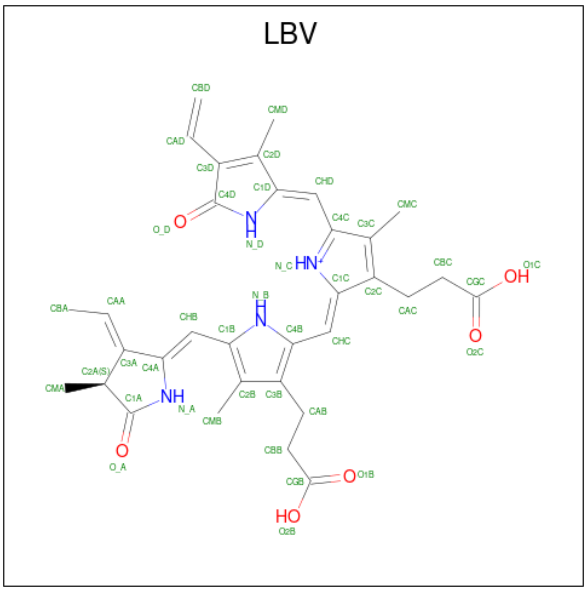
- Molecule 1 is a protein called Diguanylate cyclase (GGDEF) domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	502	Total	C	N	O	S	0	1	0
			4051	2564	719	753	15			
1	A	512	Total	C	N	O	S	0	1	0
			4129	2614	732	768	15			
1	C	509	Total	C	N	O	S	0	3	0
			4124	2614	736	759	15			
1	B	490	Total	C	N	O	S	0	3	0
			3983	2525	705	738	15			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	GLY	-	expression tag	UNP F7RW09
D	0	ALA	-	expression tag	UNP F7RW09
D	1	MET	-	expression tag	UNP F7RW09
D	2	ALA	-	expression tag	UNP F7RW09
A	-1	GLY	-	expression tag	UNP F7RW09
A	0	ALA	-	expression tag	UNP F7RW09
A	1	MET	-	expression tag	UNP F7RW09
A	2	ALA	-	expression tag	UNP F7RW09
C	-1	GLY	-	expression tag	UNP F7RW09
C	0	ALA	-	expression tag	UNP F7RW09
C	1	MET	-	expression tag	UNP F7RW09
C	2	ALA	-	expression tag	UNP F7RW09
B	-1	GLY	-	expression tag	UNP F7RW09
B	0	ALA	-	expression tag	UNP F7RW09
B	1	MET	-	expression tag	UNP F7RW09
B	2	ALA	-	expression tag	UNP F7RW09

- Molecule 2 is 3-[2-[(Z)-[3-(2-carboxyethyl)-5-[(Z)-(4-ethenyl-3-methyl-5-oxidanylidene-pyrrol-2-ylidene)methyl]-4-methyl-pyrrol-1-ium -2-ylidene]methyl]-5-[(Z)-[(3E)-3-ethylidene-4-methyl-5-oxidanylidene-pyrrolidin-2-ylidene]methyl]-4-methyl-1H-pyrrol-3- yl]propanoic acid (three-letter code: LBV) (formula: $C_{33}H_{37}N_4O_6$).

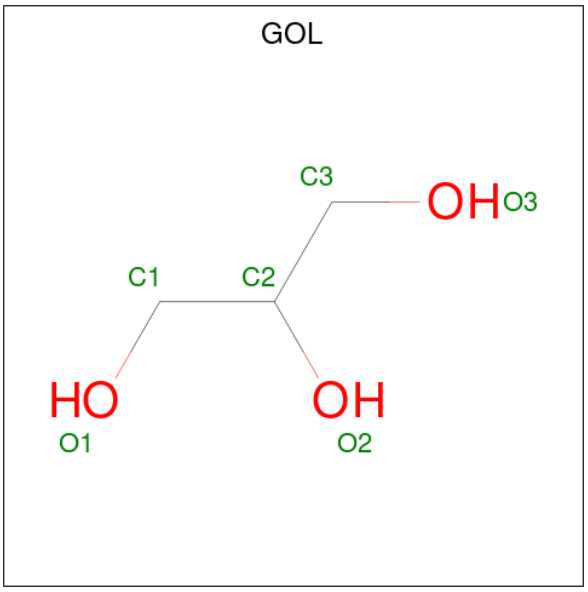


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total C N O 43 33 4 6	0	0
2	A	1	Total C N O 43 33 4 6	0	0
2	C	1	Total C N O 43 33 4 6	0	0
2	B	1	Total C N O 43 33 4 6	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	2	Total Cl 2 2	0	0
3	A	2	Total Cl 2 2	0	0
3	C	2	Total Cl 2 2	0	0
3	B	2	Total Cl 2 2	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0

- Molecule 5 is water.

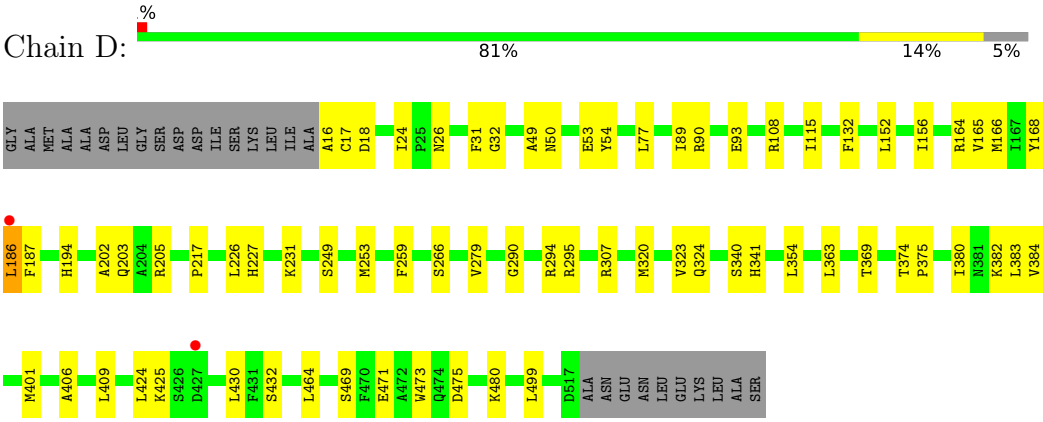
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	99	Total O 99 99	0	0
5	A	79	Total O 79 79	0	0
5	C	84	Total O 84 84	0	0
5	B	92	Total O 92 92	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

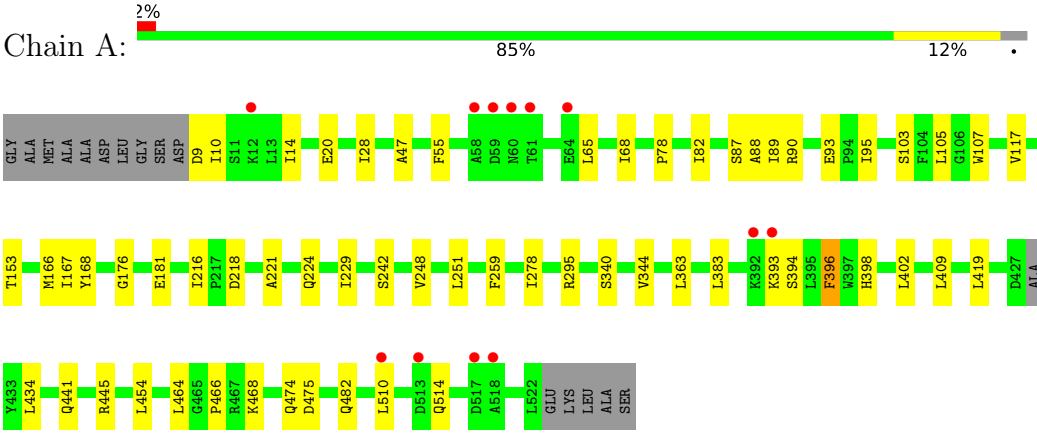
• Molecule 1: Diguanylate cyclase (GGDEF) domain-containing protein

Chain D:



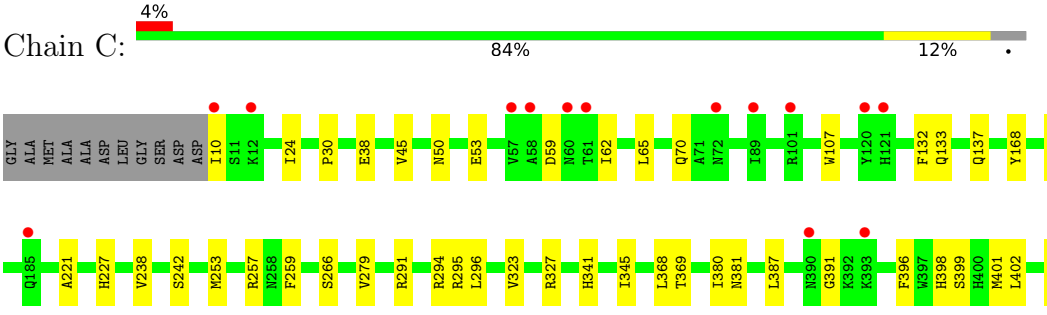
• Molecule 1: Diguanylate cyclase (GGDEF) domain-containing protein

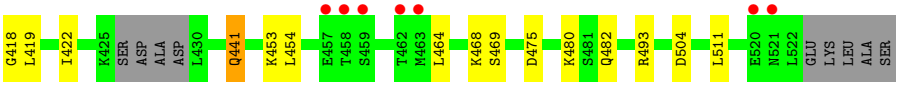
Chain A:



• Molecule 1: Diguanylate cyclase (GGDEF) domain-containing protein

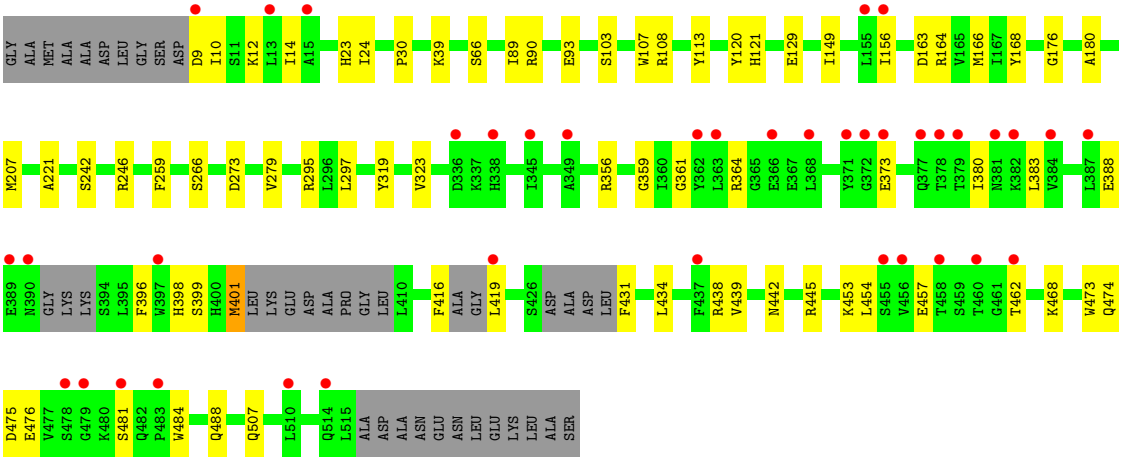
Chain C:





• Molecule 1: Diguanylate cyclase (GGDEF) domain-containing protein

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	83.50Å 129.00Å 122.01Å 90.00° 96.34° 90.00°	Depositor
Resolution (Å)	48.13 – 2.40 48.13 – 2.40	Depositor EDS
% Data completeness (in resolution range)	93.0 (48.13-2.40) 93.0 (48.13-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.56 (at 2.39Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.177 , 0.230 0.178 , 0.231	Depositor DCC
R_{free} test set	4668 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	48.8	Xtriage
Anisotropy	0.395	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 41.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	16833	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, GOL, LBV

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.39	1/4227 (0.0%)	0.56	0/5741
1	B	0.39	0/4083	0.56	0/5543
1	C	0.38	0/4229	0.56	0/5742
1	D	0.40	0/4150	0.58	1/5639 (0.0%)
All	All	0.39	1/16689 (0.0%)	0.56	1/22665 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	20	GLU	C-N	6.89	1.47	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	186	LEU	CA-CB-CG	5.40	127.72	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4129	0	4063	33	0
1	B	3983	0	3913	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	4124	0	4075	33	0
1	D	4051	0	3978	41	0
2	A	43	0	34	1	0
2	B	43	0	33	2	0
2	C	43	0	34	0	0
2	D	43	0	35	4	0
3	A	2	0	0	0	0
3	B	2	0	0	1	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	6	0	8	1	0
4	C	6	0	8	1	0
5	A	79	0	0	1	0
5	B	92	0	0	1	0
5	C	84	0	0	2	0
5	D	99	0	0	0	0
All	All	16833	0	16181	151	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (151) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:17:CYS:SG	2:D:601:LBV:HBA3	1.24	1.71
1:D:17:CYS:HG	2:D:601:LBV:HBA3	1.23	0.94
1:B:399:SER:OG	1:B:401:MET:SD	2.44	0.75
1:B:380:ILE:HA	1:B:383:LEU:HD12	1.71	0.73
1:D:17:CYS:SG	2:D:601:LBV:HBA1	2.30	0.69
1:D:424:LEU:HB2	1:D:432:SER:HB3	1.75	0.68
1:C:10:ILE:HD12	1:C:453:LYS:HE3	1.77	0.67
1:C:504:ASP:OD2	5:C:701:HOH:O	2.15	0.65
1:B:398:HIS:HA	1:B:419:LEU:O	1.97	0.64
1:D:473:TRP:CZ3	1:D:475:ASP:HB3	2.34	0.62
2:B:601:LBV:N_D	2:B:601:LBV:HMC1	2.15	0.60
1:C:454:LEU:HD21	1:C:468:LYS:HE3	1.84	0.60
1:C:381:ASN:OD1	1:B:89:ILE:HG21	2.02	0.59
1:D:374:THR:HG22	1:D:375:PRO:O	2.01	0.59
1:B:163:ASP:OD2	5:B:701:HOH:O	2.17	0.58
1:B:89:ILE:O	1:B:108:ARG:NH2	2.37	0.58
1:A:103:SER:HB2	1:A:120:TYR:HB2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:LEU:HD22	1:A:466:PRO:HD3	1.85	0.58
1:B:207:MET:HG2	1:B:246:ARG:NH2	2.19	0.57
1:D:26:ASN:HA	1:D:226:LEU:HD12	1.87	0.57
1:C:107:TRP:CE2	1:C:242:SER:HB2	2.40	0.57
1:A:65:LEU:HD12	1:A:68:ILE:HD12	1.89	0.55
1:A:14:ILE:HG12	1:A:464:LEU:HD22	1.89	0.54
1:B:107:TRP:CE2	1:B:242:SER:HB2	2.42	0.54
2:D:601:LBV:N_D	2:D:601:LBV:HMC1	2.24	0.53
1:B:168:TYR:CZ	1:B:176:GLY:HA3	2.42	0.53
1:B:356:ARG:HD2	1:B:488:GLN:HE22	1.73	0.53
1:A:216:ILE:HG12	1:A:248:VAL:HG21	1.91	0.52
1:D:341:HIS:HD2	1:D:369:THR:OG1	1.93	0.51
1:D:406:ALA:HB1	1:D:409:LEU:HD12	1.92	0.51
1:D:32:GLY:HA2	1:D:54:TYR:CZ	2.46	0.51
1:A:168:TYR:CZ	1:A:176:GLY:HA3	2.45	0.51
1:B:454:LEU:HD11	1:B:468:LYS:HE3	1.93	0.51
1:D:383:LEU:HD23	1:D:409:LEU:HD13	1.93	0.50
1:D:382:LYS:HG2	1:D:409:LEU:HD22	1.94	0.50
1:B:356:ARG:HB2	1:B:438:ARG:HH21	1.77	0.50
1:D:16:ALA:HB3	1:D:464:LEU:HD11	1.93	0.49
1:D:266:SER:HA	1:D:279:VAL:O	2.13	0.49
1:C:291:ARG:O	1:C:295:ARG:HG2	2.12	0.49
1:D:295:ARG:HH11	1:D:295:ARG:HG3	1.78	0.48
1:C:171:ASP:OD2	1:C:175:ASN:HB2	2.12	0.48
1:B:39:LYS:HG3	1:B:113:TYR:CZ	2.48	0.48
1:D:90:ARG:HB2	1:D:93:GLU:OE1	2.13	0.48
1:D:164:ARG:HD3	1:D:166:MET:SD	2.53	0.48
1:A:441:GLN:OE1	1:A:482:GLN:NE2	2.46	0.48
1:D:320:MET:O	1:D:324:GLN:HG2	2.13	0.48
2:A:601:LBV:N_D	2:A:601:LBV:HMC1	2.28	0.48
1:B:164:ARG:HD3	1:B:166:MET:HE1	1.94	0.48
1:D:156:ILE:HB	1:D:165:VAL:HG11	1.96	0.48
1:C:59:ASP:HB3	1:C:62:ILE:HG12	1.96	0.48
1:D:374:THR:CG2	1:D:380:ILE:HD11	2.44	0.48
1:D:177:ARG:HD3	1:D:194:HIS:NE2	2.29	0.47
1:A:87:SER:O	1:A:89:ILE:HG13	2.14	0.47
1:D:49:ALA:HB2	1:D:227:HIS:CD2	2.49	0.47
1:B:416:PHE:HA	1:B:439:VAL:HA	1.95	0.47
1:A:394:SER:HB2	1:A:396:PHE:O	2.14	0.47
1:C:341[A]:HIS:ND1	1:C:369:THR:OG1	2.37	0.47
1:B:156:ILE:HG23	1:B:297:LEU:HD22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:454:LEU:HD11	1:A:468:LYS:HE3	1.96	0.47
1:C:65:LEU:HD21	1:C:227:HIS:CG	2.49	0.47
1:D:152:LEU:O	1:D:156:ILE:HG12	2.15	0.46
1:A:153:THR:HG22	1:A:167:ILE:HG13	1.97	0.46
1:B:398:HIS:HB2	1:B:484:TRP:CD1	2.50	0.46
1:D:363:LEU:HD13	1:D:384:VAL:HG21	1.98	0.46
1:A:383:LEU:HD23	1:A:409:LEU:HG	1.97	0.46
1:C:133:GLN:O	1:C:137:GLN:HG3	2.15	0.46
1:A:78:PRO:O	1:A:82:ILE:HG13	2.16	0.46
1:B:361:GLY:O	1:B:434:LEU:HD12	2.15	0.46
1:A:393:LYS:HE3	1:A:393:LYS:HB2	1.82	0.45
1:B:359:GLY:HA3	1:B:373:GLU:O	2.17	0.45
1:B:10:ILE:HG12	1:B:453:LYS:HE2	1.98	0.45
1:C:168:TYR:CZ	1:C:176:GLY:HA3	2.52	0.45
1:B:129:GLU:OE1	1:B:129:GLU:N	2.44	0.45
1:C:323:VAL:O	1:C:327:ARG:HG3	2.17	0.45
1:D:50:ASN:O	1:D:53:GLU:HG2	2.16	0.45
1:D:425:LYS:HG3	1:D:430:LEU:HD12	1.99	0.44
1:A:402:LEU:HD11	1:A:419:LEU:HB2	1.99	0.44
1:A:132:PHE:CD2	4:A:604:GOL:H32	2.52	0.44
1:C:50:ASN:O	1:C:53:GLU:HG2	2.17	0.44
1:B:442:ASN:ND2	1:B:476:GLU:OE2	2.38	0.44
1:B:445:ARG:O	1:B:474:GLN:HA	2.18	0.44
1:B:473:TRP:CZ3	1:B:475:ASP:HB3	2.53	0.44
1:C:402:LEU:HD13	1:C:410:LEU:HD11	2.00	0.44
1:B:10:ILE:O	1:B:14:ILE:HG13	2.18	0.44
1:D:469:SER:OG	1:D:471:GLU:HG3	2.18	0.43
1:A:28:ILE:HG13	1:A:224:GLN:HB2	2.00	0.43
1:A:55:PHE:CZ	1:A:117:VAL:HG21	2.53	0.43
1:B:9:ASP:HB3	1:B:12:LYS:HD2	2.00	0.43
1:A:166:MET:HG2	1:A:181:GLU:HG3	2.00	0.43
1:C:132:PHE:CZ	1:C:296:LEU:HA	2.53	0.43
1:B:23:HIS:CD2	1:B:24:ILE:HG23	2.53	0.43
1:B:90:ARG:NE	1:B:93:GLU:OE1	2.35	0.43
1:C:291:ARG:HA	1:C:294:ARG:HD2	2.00	0.43
1:A:107:TRP:CE2	1:A:242:SER:HB2	2.53	0.43
1:B:388:GLU:HG3	1:B:431:PHE:CZ	2.54	0.43
1:A:398:HIS:HA	1:A:419:LEU:O	2.19	0.43
1:D:89:ILE:O	1:D:108:ARG:NH2	2.52	0.43
1:C:454:LEU:O	1:C:464:LEU:HD12	2.19	0.43
1:B:149:ILE:HD12	1:B:180:ALA:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:319:TYR:O	1:B:323:VAL:HG23	2.18	0.43
1:A:445:ARG:NH2	1:A:475:ASP:OD2	2.42	0.43
1:C:401:MET:SD	1:C:480:LYS:HE2	2.59	0.42
1:B:457:GLU:OE1	1:B:462:THR:HG22	2.18	0.42
1:A:340:SER:O	1:A:344:VAL:HG23	2.20	0.42
1:A:510:LEU:HG	1:A:514:GLN:HE21	1.83	0.42
1:B:266:SER:HA	1:B:279:VAL:O	2.19	0.42
1:D:202:ALA:HA	1:D:205:ARG:NH1	2.35	0.42
1:A:218:ASP:HB3	1:A:221:ALA:HB2	2.00	0.42
1:A:434:LEU:HD12	1:A:434:LEU:HA	1.89	0.42
1:C:38:GLU:HG3	1:C:45:VAL:HG11	2.01	0.42
1:D:290:GLY:O	1:D:294:ARG:HG3	2.20	0.42
1:C:398:HIS:HA	1:C:419:LEU:O	2.20	0.42
1:D:401:MET:HG2	1:D:480:LYS:HG2	2.02	0.42
1:C:24:ILE:HG22	1:C:238:VAL:O	2.19	0.42
1:C:368:LEU:HD21	1:C:380:ILE:HD12	2.00	0.42
1:D:31:PHE:CD1	1:D:217:PRO:HG2	2.54	0.42
1:D:231:LYS:HE2	1:D:231:LYS:HB3	1.73	0.42
1:A:47:ALA:HB3	1:A:229:ILE:HD11	2.01	0.42
1:B:120:TYR:CG	1:B:121:HIS:N	2.88	0.42
1:A:90:ARG:HD2	1:A:93:GLU:OE2	2.20	0.41
1:D:168:TYR:CZ	1:D:176:GLY:HA3	2.55	0.41
1:B:438:ARG:HB3	1:B:481:SER:HB2	2.02	0.41
1:C:266:SER:HA	1:C:279:VAL:O	2.20	0.41
1:C:387:LEU:O	1:C:391:GLY:N	2.37	0.41
2:B:601:LBV:HMC1	2:B:601:LBV:C1D	2.50	0.41
1:D:77:LEU:HD11	1:D:115:ILE:HD13	2.02	0.41
1:A:9:ASP:OD1	1:A:10:ILE:N	2.53	0.41
1:A:95:ILE:O	1:A:105:LEU:HA	2.20	0.41
1:C:253:MET:O	1:C:257:ARG:HG3	2.19	0.41
1:C:441:GLN:OE1	1:C:482:GLN:NE2	2.51	0.41
1:D:132:PHE:CD2	4:C:604:GOL:H12	2.55	0.41
1:A:295:ARG:NH2	5:A:706:HOH:O	2.48	0.41
1:A:363:LEU:O	1:A:432:SER:HA	2.21	0.41
1:B:103:SER:HB2	1:B:120:TYR:HB2	2.03	0.41
1:D:323:VAL:HG22	1:D:354:LEU:HD11	2.01	0.41
1:D:177:ARG:HD3	1:D:194:HIS:CE1	2.56	0.41
1:C:30:PRO:CG	1:C:221:ALA:HB1	2.51	0.41
1:C:493:ARG:HD3	5:C:776:HOH:O	2.22	0.40
1:B:438:ARG:HD2	1:B:484:TRP:CZ2	2.56	0.40
1:C:345:ILE:HD13	1:C:345:ILE:HA	1.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:511:LEU:HA	1:C:511:LEU:HD23	1.89	0.40
1:B:364:ARG:NH2	1:B:507:GLN:OE1	2.51	0.40
1:D:90:ARG:HE	1:D:93:GLU:CD	2.23	0.40
1:A:409:LEU:HD12	1:A:409:LEU:HA	1.91	0.40
1:C:422:ILE:HG21	1:C:493:ARG:HA	2.03	0.40
1:D:18:ASP:HA	1:D:203:GLN:OE1	2.22	0.40
1:B:30:PRO:HG3	1:B:221:ALA:HB1	2.03	0.40
1:B:295:ARG:NH1	3:B:602:CL:CL	2.88	0.40
1:D:340:SER:HB2	1:D:499:LEU:HD22	2.03	0.40
1:C:399:SER:O	1:C:418:GLY:HA2	2.22	0.40
1:B:295:ARG:HH11	1:B:295:ARG:HG3	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	509/529 (96%)	497 (98%)	11 (2%)	1 (0%)	47 62
1	B	483/529 (91%)	473 (98%)	10 (2%)	0	100 100
1	C	508/529 (96%)	494 (97%)	14 (3%)	0	100 100
1	D	501/529 (95%)	488 (97%)	13 (3%)	0	100 100
All	All	2001/2116 (95%)	1952 (98%)	48 (2%)	1 (0%)	51 100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	88	ALA

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	448/457 (98%)	444 (99%)	4 (1%)	78	90
1	B	435/457 (95%)	430 (99%)	5 (1%)	73	87
1	C	447/457 (98%)	441 (99%)	6 (1%)	69	84
1	D	439/457 (96%)	431 (98%)	8 (2%)	59	76
All	All	1769/1828 (97%)	1746 (99%)	23 (1%)	69	84

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	24	ILE
1	D	186	LEU
1	D	187	PHE
1	D	249	SER
1	D	253	MET
1	D	259	PHE
1	D	307	ARG
1	D	396	PHE
1	A	259	PHE
1	A	278	ILE
1	A	396	PHE
1	A	474	GLN
1	C	70	GLN
1	C	259	PHE
1	C	396	PHE
1	C	441	GLN
1	C	469	SER
1	C	475	ASP
1	B	66	SER
1	B	259	PHE
1	B	273	ASP
1	B	396	PHE
1	B	401	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	121	HIS
1	D	123	GLN
1	D	341	HIS
1	D	441	GLN
1	D	482	GLN
1	A	441	GLN
1	A	482	GLN
1	B	121	HIS
1	B	123	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 14 ligands modelled in this entry, 8 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	GOL	C	604	-	5,5,5	0.36	0	5,5,5	0.27	0
4	GOL	A	604	-	5,5,5	0.39	0	5,5,5	0.49	0
2	LBV	B	601	1	42,46,46	2.45	15 (35%)	47,67,67	1.73	8 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	LBV	A	601	1	42,46,46	2.68	12 (28%)	47,67,67	1.73	9 (19%)
2	LBV	D	601	1	42,46,46	2.53	14 (33%)	47,67,67	1.58	10 (21%)
2	LBV	C	601	1	42,46,46	2.57	14 (33%)	47,67,67	1.71	12 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	C	604	-	-	1/4/4/4	-
4	GOL	A	604	-	-	3/4/4/4	-
2	LBV	B	601	1	-	8/26/74/74	0/4/4/4
2	LBV	A	601	1	-	8/26/74/74	0/4/4/4
2	LBV	D	601	1	-	8/26/74/74	0/4/4/4
2	LBV	C	601	1	-	8/26/74/74	0/4/4/4

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	LBV	C2A-C1A	-7.20	1.43	1.51
2	B	601	LBV	C2A-C3A	-6.80	1.42	1.51
2	B	601	LBV	C2A-C1A	-6.80	1.43	1.51
2	D	601	LBV	C2A-C1A	-6.75	1.43	1.51
2	A	601	LBV	C2A-C1A	-6.67	1.43	1.51
2	A	601	LBV	CHC-C1C	6.63	1.40	1.35
2	A	601	LBV	CAB-C3B	-6.46	1.42	1.52
2	D	601	LBV	C2A-C3A	-6.29	1.43	1.51
2	D	601	LBV	CAB-C3B	-5.42	1.44	1.52
2	A	601	LBV	C2A-C3A	-5.41	1.44	1.51
2	B	601	LBV	CAB-C3B	-5.25	1.44	1.52
2	A	601	LBV	CMB-C2B	-5.03	1.41	1.51
2	C	601	LBV	C2A-C3A	-5.00	1.45	1.51
2	C	601	LBV	CMD-C2D	-4.86	1.40	1.50
2	D	601	LBV	CHC-C1C	4.84	1.39	1.35
2	C	601	LBV	CMB-C2B	-4.79	1.41	1.51
2	C	601	LBV	CHC-C1C	4.72	1.39	1.35
2	A	601	LBV	CMC-C3C	-4.42	1.41	1.50
2	D	601	LBV	CMB-C2B	-4.26	1.42	1.51
2	C	601	LBV	CMC-C3C	-4.25	1.41	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	LBV	CAB-C3B	-4.19	1.45	1.52
2	D	601	LBV	CMC-C3C	-4.17	1.42	1.50
2	A	601	LBV	CMD-C2D	-3.94	1.42	1.50
2	B	601	LBV	CMC-C3C	-3.83	1.42	1.50
2	B	601	LBV	CMB-C2B	-3.68	1.44	1.51
2	A	601	LBV	CMA-C2A	-3.64	1.42	1.53
2	D	601	LBV	CMD-C2D	-3.61	1.43	1.50
2	D	601	LBV	CMA-C2A	-3.56	1.42	1.53
2	B	601	LBV	CMD-C2D	-3.55	1.43	1.50
2	C	601	LBV	CMA-C2A	-3.43	1.42	1.53
2	B	601	LBV	CMA-C2A	-3.42	1.42	1.53
2	C	601	LBV	CAA-C3A	3.33	1.42	1.33
2	A	601	LBV	CAA-C3A	3.18	1.42	1.33
2	C	601	LBV	CHB-C4A	3.13	1.40	1.34
2	C	601	LBV	CAC-C2C	-3.05	1.43	1.51
2	D	601	LBV	CBB-CGB	-3.05	1.43	1.50
2	C	601	LBV	CBB-CGB	-3.03	1.43	1.50
2	C	601	LBV	C1D-C2D	-2.77	1.40	1.45
2	D	601	LBV	CAA-C3A	2.70	1.40	1.33
2	B	601	LBV	C4A-C3A	-2.69	1.40	1.45
2	B	601	LBV	C4A-N-A	-2.67	1.33	1.37
2	B	601	LBV	CAC-C2C	-2.63	1.44	1.51
2	D	601	LBV	CHB-C4A	2.60	1.39	1.34
2	A	601	LBV	CBB-CGB	-2.59	1.44	1.50
2	A	601	LBV	CHB-C4A	2.57	1.39	1.34
2	B	601	LBV	CHC-C1C	2.51	1.37	1.35
2	B	601	LBV	CAA-C3A	2.49	1.40	1.33
2	B	601	LBV	CBB-CGB	-2.43	1.44	1.50
2	D	601	LBV	CAC-C2C	-2.34	1.45	1.51
2	B	601	LBV	C1C-C2C	-2.32	1.42	1.45
2	D	601	LBV	O2B-CGB	-2.30	1.23	1.30
2	D	601	LBV	CAD-C3D	-2.22	1.41	1.47
2	A	601	LBV	O2B-CGB	-2.18	1.23	1.30
2	B	601	LBV	CBA-CAA	-2.11	1.41	1.49
2	C	601	LBV	CBC-CGC	-2.03	1.45	1.50

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601	LBV	C4B-CHC-C1C	7.33	137.57	128.81
2	C	601	LBV	C4B-CHC-C1C	6.32	136.36	128.81
2	B	601	LBV	C4B-CHC-C1C	5.82	135.77	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	601	LBV	C4B-CHC-C1C	5.31	135.16	128.81
2	B	601	LBV	O-A-C1A-N-A	-4.43	119.58	124.94
2	A	601	LBV	O-A-C1A-C2A	3.55	129.71	126.28
2	C	601	LBV	O-A-C1A-N-A	-3.22	121.05	124.94
2	B	601	LBV	O-A-C1A-C2A	3.20	129.38	126.28
2	C	601	LBV	O-A-C1A-C2A	2.81	129.00	126.28
2	D	601	LBV	CHC-C1C-N-C	-2.69	125.10	128.83
2	B	601	LBV	O-D-C4D-C3D	2.66	135.48	129.46
2	B	601	LBV	CHC-C1C-N-C	-2.61	125.21	128.83
2	D	601	LBV	O-A-C1A-C2A	2.46	128.66	126.28
2	D	601	LBV	O-D-C4D-N-D	-2.43	119.43	125.08
2	B	601	LBV	O-D-C4D-N-D	-2.43	119.44	125.08
2	A	601	LBV	O-A-C1A-N-A	-2.42	122.01	124.94
2	A	601	LBV	C2C-C1C-N-C	-2.41	106.55	110.05
2	C	601	LBV	O1B-CGB-CBB	-2.36	115.50	123.08
2	A	601	LBV	CAA-C3A-C4A	-2.36	123.51	126.36
2	C	601	LBV	CMD-C2D-C1D	-2.31	121.28	124.17
2	A	601	LBV	CHC-C1C-N-C	-2.30	125.64	128.83
2	D	601	LBV	O-D-C4D-C3D	2.30	134.67	129.46
2	D	601	LBV	CBB-CAB-C3B	-2.23	108.82	112.62
2	B	601	LBV	CBB-CAB-C3B	-2.18	108.90	112.62
2	A	601	LBV	O-D-C4D-N-D	-2.17	120.03	125.08
2	C	601	LBV	O-D-C4D-C3D	2.15	134.33	129.46
2	B	601	LBV	O1B-CGB-CBB	-2.13	116.23	123.08
2	C	601	LBV	C2C-C1C-N-C	-2.12	106.97	110.05
2	C	601	LBV	CHC-C1C-N-C	-2.07	125.96	128.83
2	D	601	LBV	O-A-C1A-N-A	-2.06	122.44	124.94
2	C	601	LBV	CAA-C3A-C4A	-2.06	123.87	126.36
2	A	601	LBV	CHD-C4C-C3C	2.06	130.19	124.90
2	D	601	LBV	O2B-CGB-O1B	2.04	128.39	123.30
2	D	601	LBV	C2C-C1C-N-C	-2.02	107.10	110.05
2	D	601	LBV	CHD-C4C-C3C	2.02	130.10	124.90
2	C	601	LBV	O2C-CGC-CBC	-2.02	116.59	123.08
2	C	601	LBV	O-D-C4D-N-D	-2.02	120.38	125.08
2	C	601	LBV	CMC-C3C-C4C	2.02	128.17	125.06
2	A	601	LBV	O-D-C4D-C3D	2.01	134.02	129.46

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	604	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
2	C	601	LBV	C2D-C1D-CHD-C4C
2	D	601	LBV	D-N-C1D-CHD-C4C
2	C	601	LBV	D-N-C1D-CHD-C4C
2	B	601	LBV	D-N-C1D-CHD-C4C
2	D	601	LBV	C2D-C1D-CHD-C4C
2	B	601	LBV	C2D-C1D-CHD-C4C
2	A	601	LBV	D-N-C1D-CHD-C4C
2	D	601	LBV	C-N-C4C-CHD-C1D
2	A	601	LBV	C-N-C4C-CHD-C1D
2	C	601	LBV	C-N-C4C-CHD-C1D
2	B	601	LBV	C-N-C4C-CHD-C1D
2	D	601	LBV	C3C-C4C-CHD-C1D
2	A	601	LBV	C3C-C4C-CHD-C1D
2	C	601	LBV	C3C-C4C-CHD-C1D
2	B	601	LBV	C3C-C4C-CHD-C1D
4	A	604	GOL	O1-C1-C2-O2
2	A	601	LBV	C2D-C1D-CHD-C4C
4	C	604	GOL	O1-C1-C2-C3
4	A	604	GOL	O2-C2-C3-O3
2	C	601	LBV	CAB-CBB-CGB-O2B
2	D	601	LBV	CAB-CBB-CGB-O2B
2	D	601	LBV	CAC-CBC-CGC-O2C
2	B	601	LBV	CAC-CBC-CGC-O2C
2	D	601	LBV	CAC-CBC-CGC-O1C
2	D	601	LBV	CAB-CBB-CGB-O1B
2	C	601	LBV	CAB-CBB-CGB-O1B
2	A	601	LBV	CAB-CBB-CGB-O2B
2	B	601	LBV	CAC-CBC-CGC-O1C
2	A	601	LBV	CAC-CBC-CGC-O1C
2	B	601	LBV	CAB-CBB-CGB-O2B
2	C	601	LBV	CAC-CBC-CGC-O1C
2	B	601	LBV	CAB-CBB-CGB-O1B
2	A	601	LBV	CAB-CBB-CGB-O1B
2	C	601	LBV	CAC-CBC-CGC-O2C
2	A	601	LBV	CAC-CBC-CGC-O2C

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	604	GOL	1	0
4	A	604	GOL	1	0

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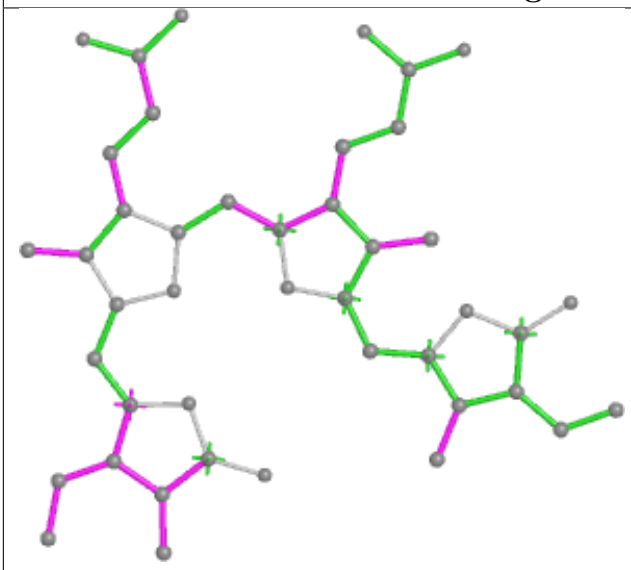
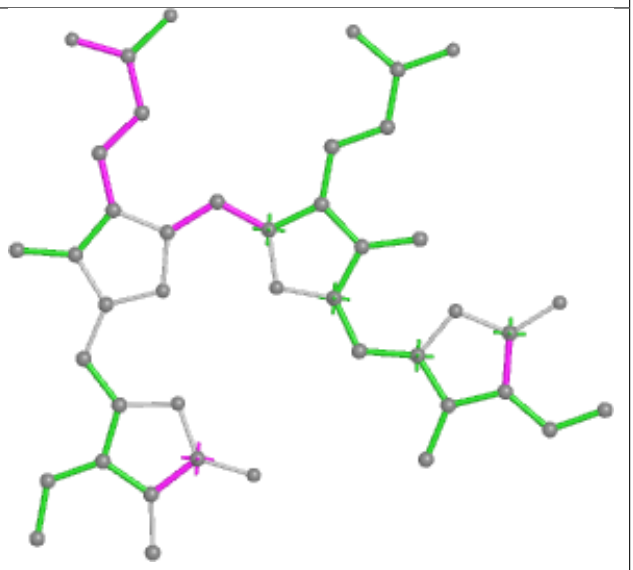
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	LBV	2	0
2	A	601	LBV	1	0
2	D	601	LBV	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

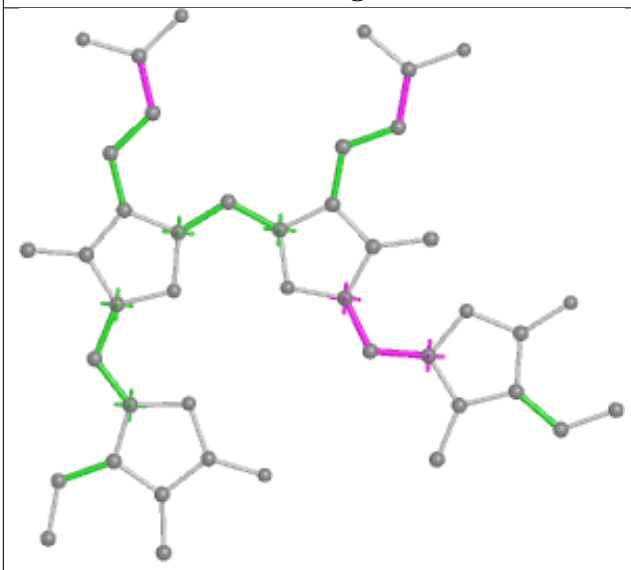
Ligand LBV B 601



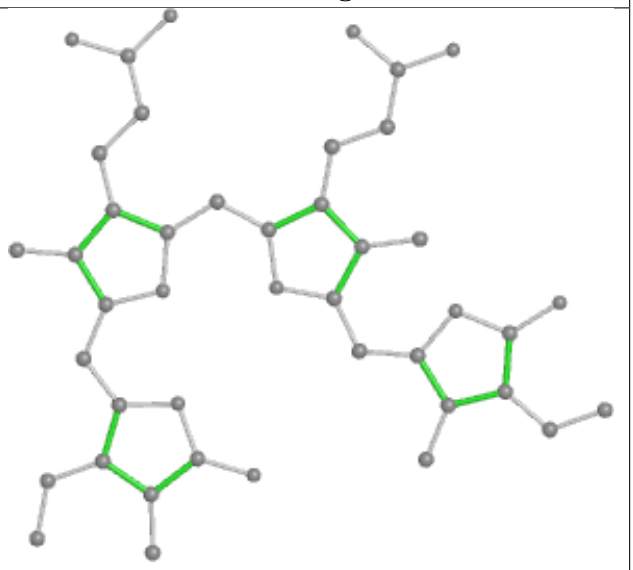
Bond lengths



Bond angles

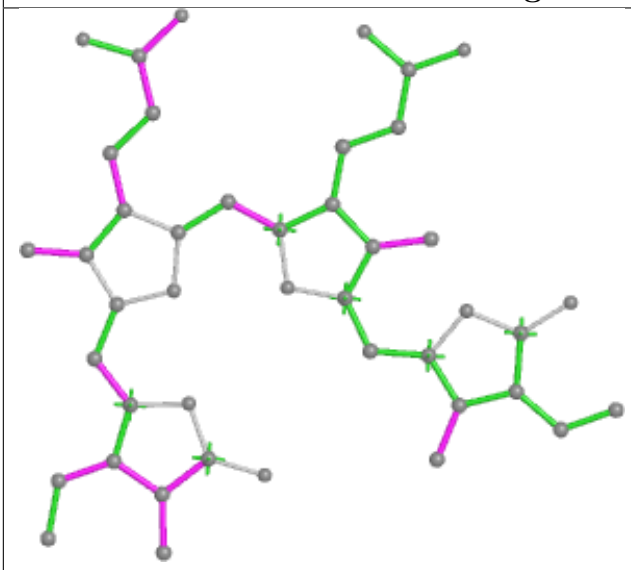


Torsions

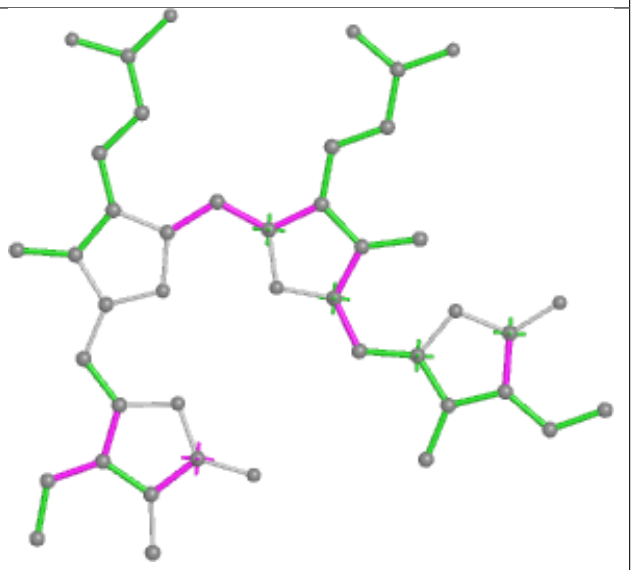


Rings

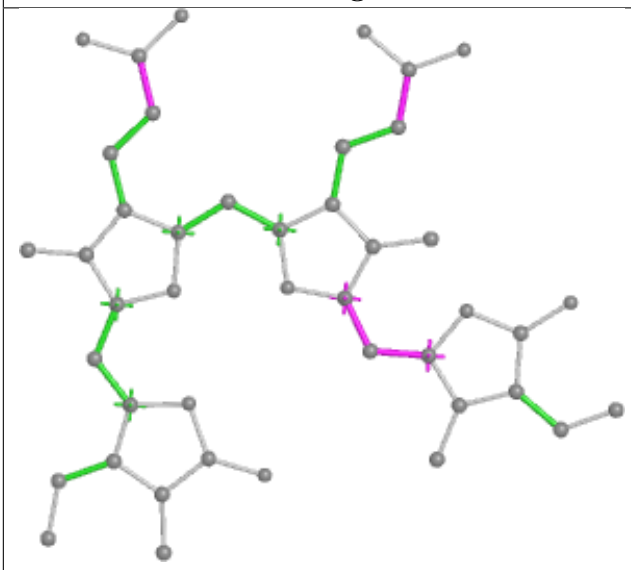
Ligand LBV A 601



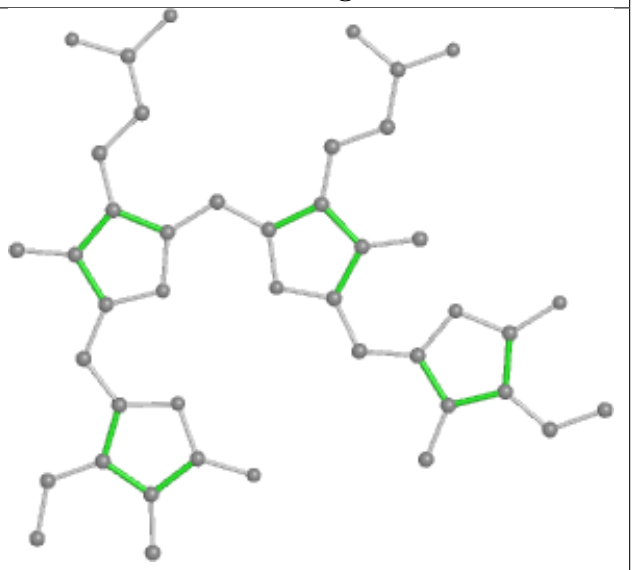
Bond lengths



Bond angles

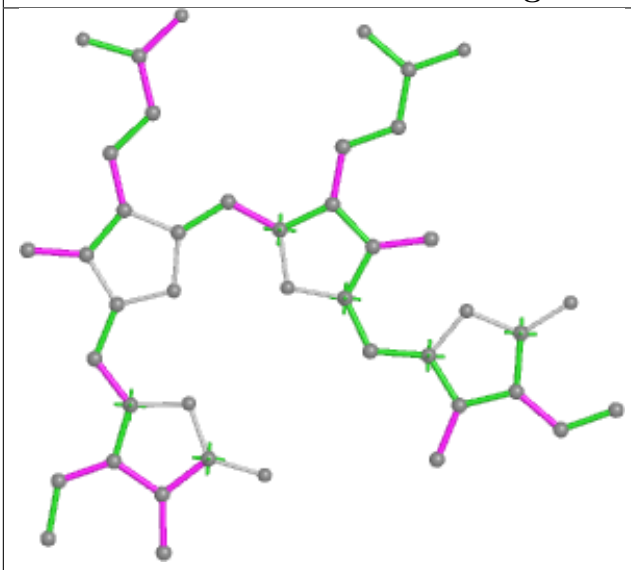


Torsions

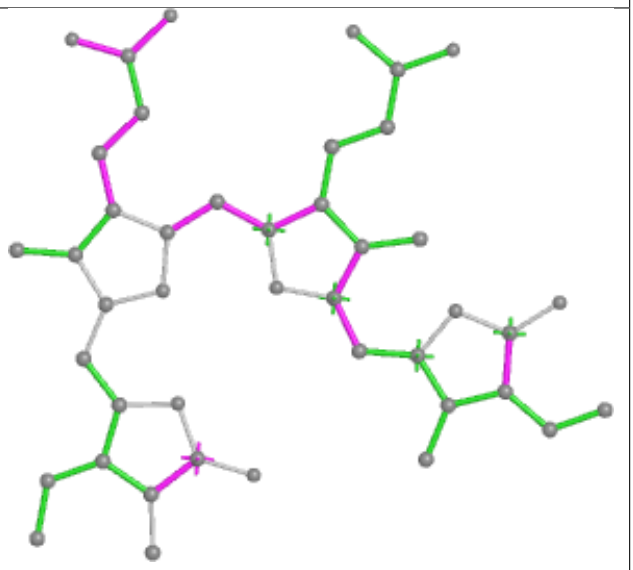


Rings

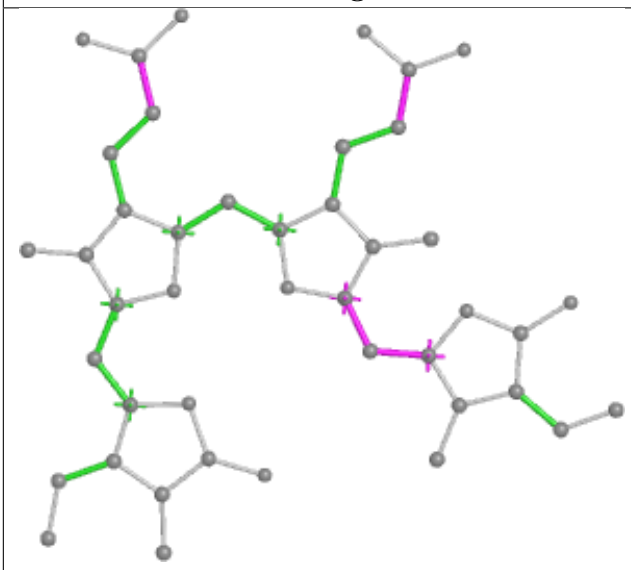
Ligand LBV D 601



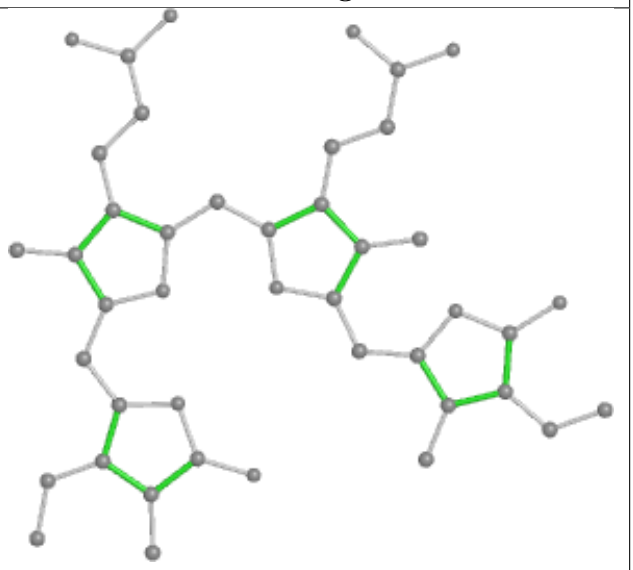
Bond lengths



Bond angles

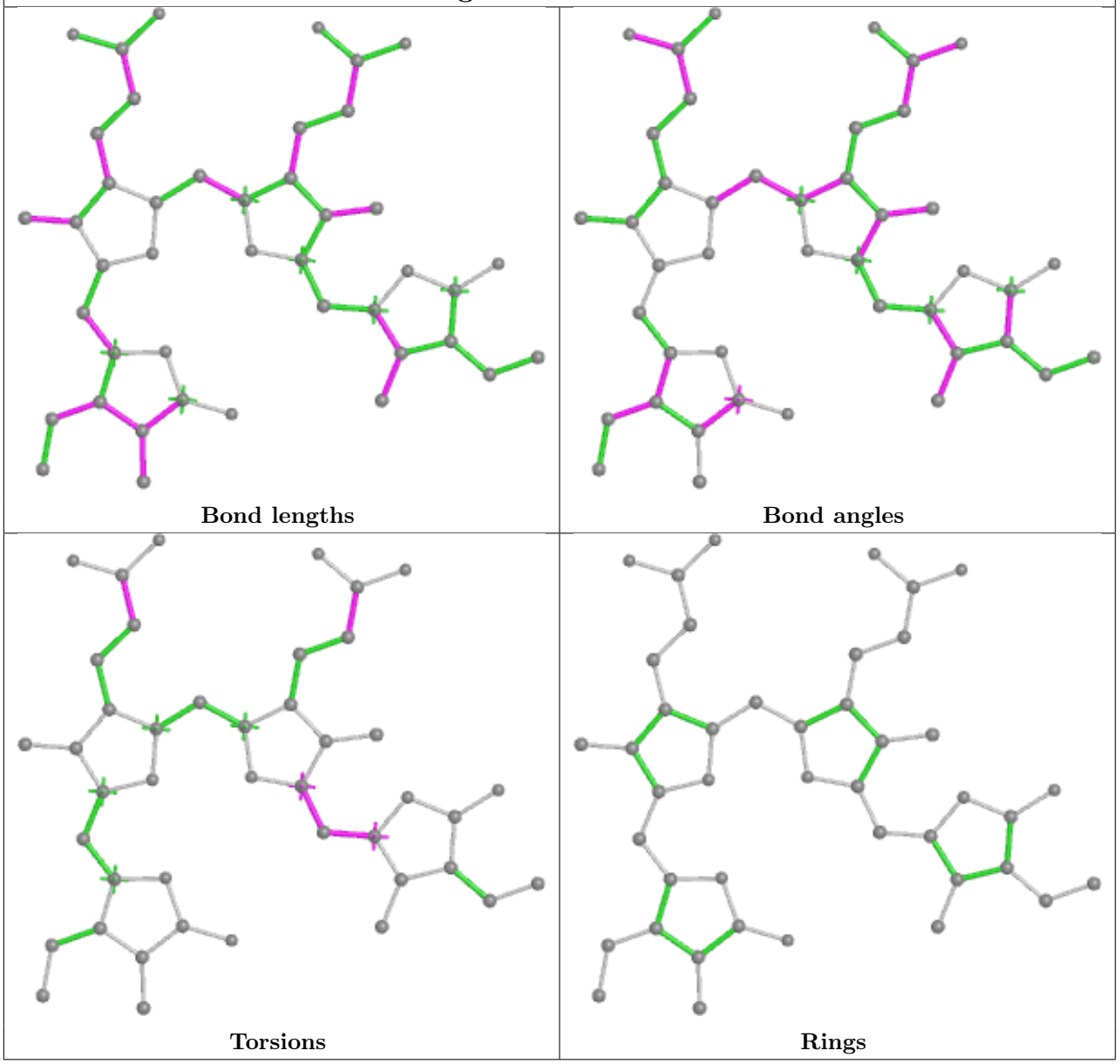


Torsions



Rings

Ligand LBV C 601



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	512/529 (96%)	0.02	12 (2%)	60	58	31, 55, 96, 128	0
1	B	490/529 (92%)	0.44	39 (7%)	12	11	31, 56, 99, 117	0
1	C	509/529 (96%)	0.06	22 (4%)	35	33	31, 55, 96, 132	0
1	D	502/529 (94%)	0.04	3 (0%)	89	88	32, 50, 86, 103	0
All	All	2013/2116 (95%)	0.14	76 (3%)	40	39	31, 54, 95, 132	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	336	ASP	4.7
1	C	10	ILE	4.3
1	B	345	ILE	4.3
1	C	390	ASN	4.2
1	B	378	THR	4.2
1	C	459	SER	3.9
1	B	456	VAL	3.8
1	B	437	PHE	3.7
1	B	368	LEU	3.6
1	A	61	THR	3.6
1	A	60	ASN	3.3
1	B	381	ASN	3.2
1	C	89	ILE	3.2
1	C	520	GLU	3.1
1	C	121	HIS	3.1
1	B	366	GLU	3.0
1	B	458	THR	2.9
1	C	521	ASN	2.9
1	A	510	LEU	2.9
1	C	60	ASN	2.9
1	B	397	TRP	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	393	LYS	2.8
1	A	392	LYS	2.8
1	C	61	THR	2.8
1	B	462	THR	2.8
1	C	12	LYS	2.7
1	B	419	LEU	2.7
1	B	481	SER	2.7
1	A	58	ALA	2.6
1	B	390	ASN	2.6
1	B	384	VAL	2.6
1	B	363	LEU	2.6
1	B	478	SER	2.6
1	C	393	LYS	2.6
1	D	427	ASP	2.6
1	B	460	THR	2.5
1	C	72	ASN	2.5
1	B	377	GLN	2.5
1	B	362	TYR	2.5
1	B	514	GLN	2.4
1	B	9	ASP	2.4
1	B	483	PRO	2.4
1	B	510	LEU	2.4
1	C	101	ARG	2.4
1	B	349	ALA	2.4
1	A	517	ASP	2.4
1	A	518	ALA	2.4
1	B	455	SER	2.4
1	B	379	THR	2.4
1	B	15	ALA	2.3
1	C	462	THR	2.3
1	D	186	LEU	2.3
1	A	59	ASP	2.3
1	C	120	TYR	2.3
1	B	372	GLY	2.3
1	C	458	THR	2.3
1	B	338	HIS	2.2
1	C	185	GLN	2.2
1	B	389	GLU	2.2
1	C	412	ASP	2.2
1	B	371	TYR	2.2
1	A	513	ASP	2.2
1	C	463	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	156	ILE	2.2
1	C	57	VAL	2.1
1	A	64	GLU	2.1
1	B	13	LEU	2.1
1	B	382	LYS	2.1
1	C	457	GLU	2.1
1	B	373	GLU	2.1
1	C	58	ALA	2.1
1	A	12	LYS	2.1
1	B	479	GLY	2.1
1	B	155	LEU	2.1
1	A	393	LYS	2.1
1	B	387	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CL	A	603	1/1	0.79	0.35	90,90,90,90	0
2	LBV	C	601	43/43	0.92	0.16	38,50,56,68	0
2	LBV	A	601	43/43	0.93	0.15	44,56,65,69	0
2	LBV	B	601	43/43	0.95	0.13	33,40,45,53	0
2	LBV	D	601	43/43	0.95	0.15	33,39,50,56	0
4	GOL	A	604	6/6	0.95	0.21	38,54,54,60	0
3	CL	D	602	1/1	0.96	0.23	52,52,52,52	0
4	GOL	C	604	6/6	0.96	0.17	46,57,61,63	0
3	CL	C	603	1/1	0.97	0.14	80,80,80,80	0
3	CL	C	602	1/1	0.98	0.19	54,54,54,54	0

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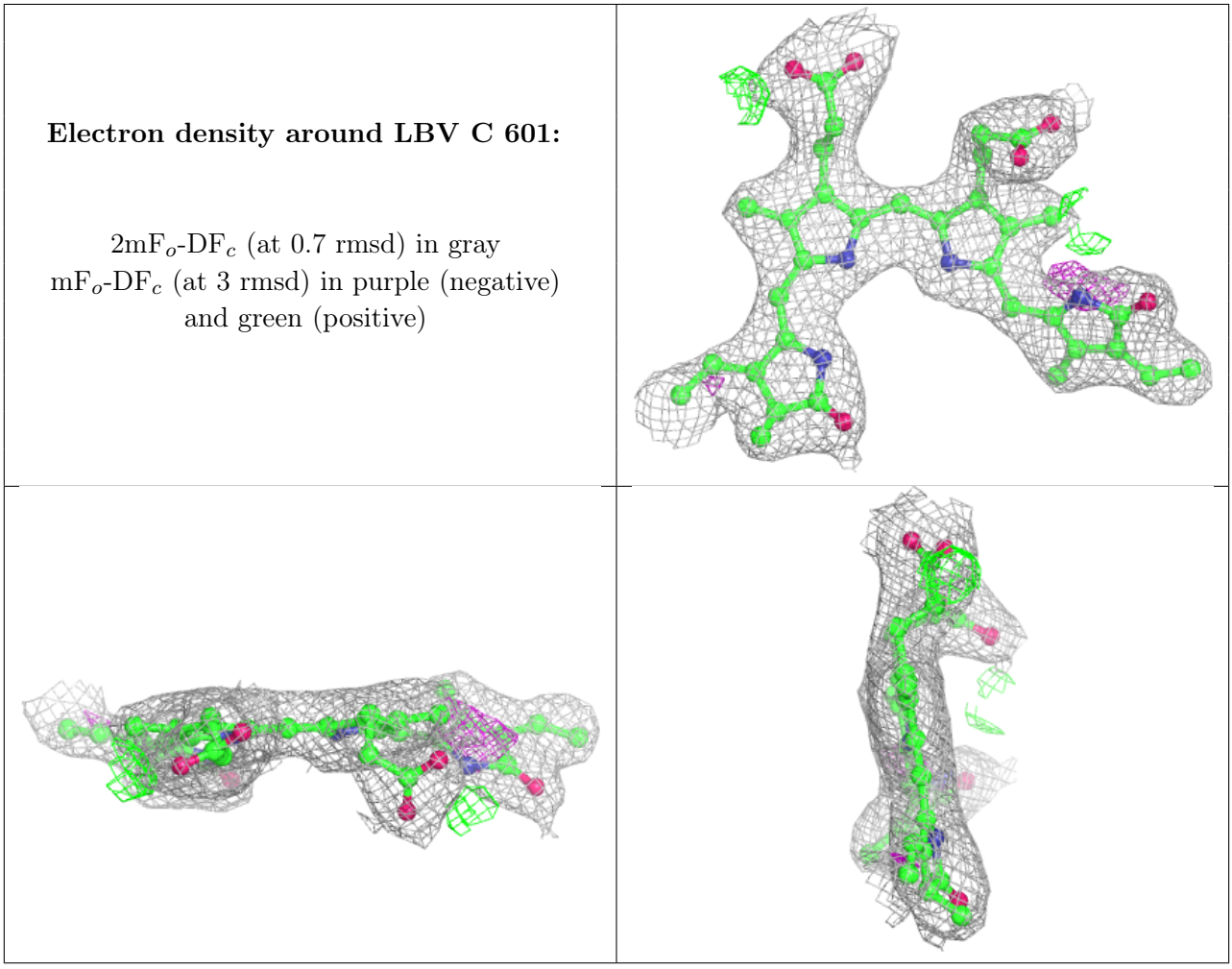
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CL	B	603	1/1	0.98	0.14	43,43,43,43	0
3	CL	A	602	1/1	0.99	0.15	42,42,42,42	0
3	CL	D	603	1/1	0.99	0.20	37,37,37,37	0
3	CL	B	602	1/1	0.99	0.24	40,40,40,40	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

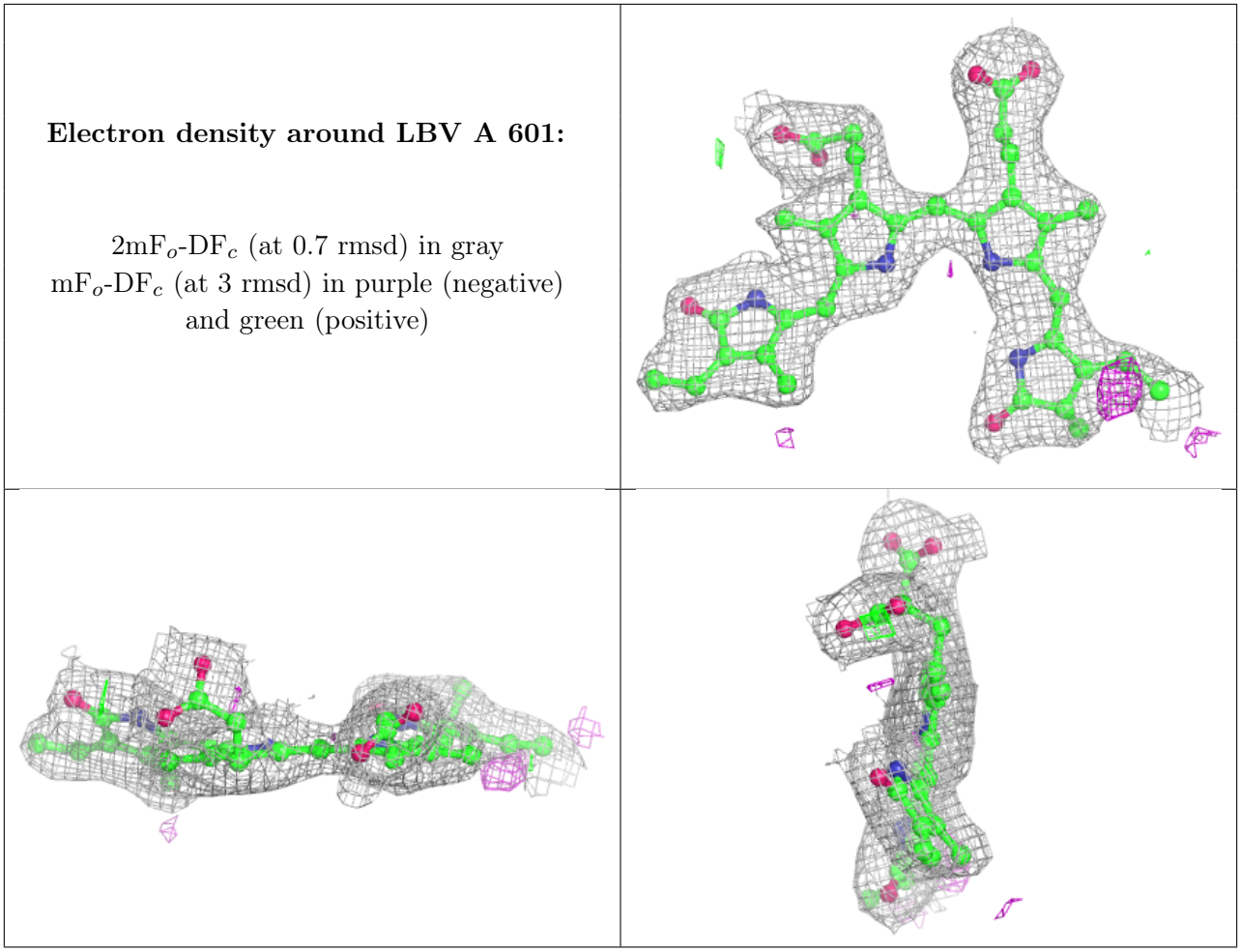
Electron density around LBV C 601:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



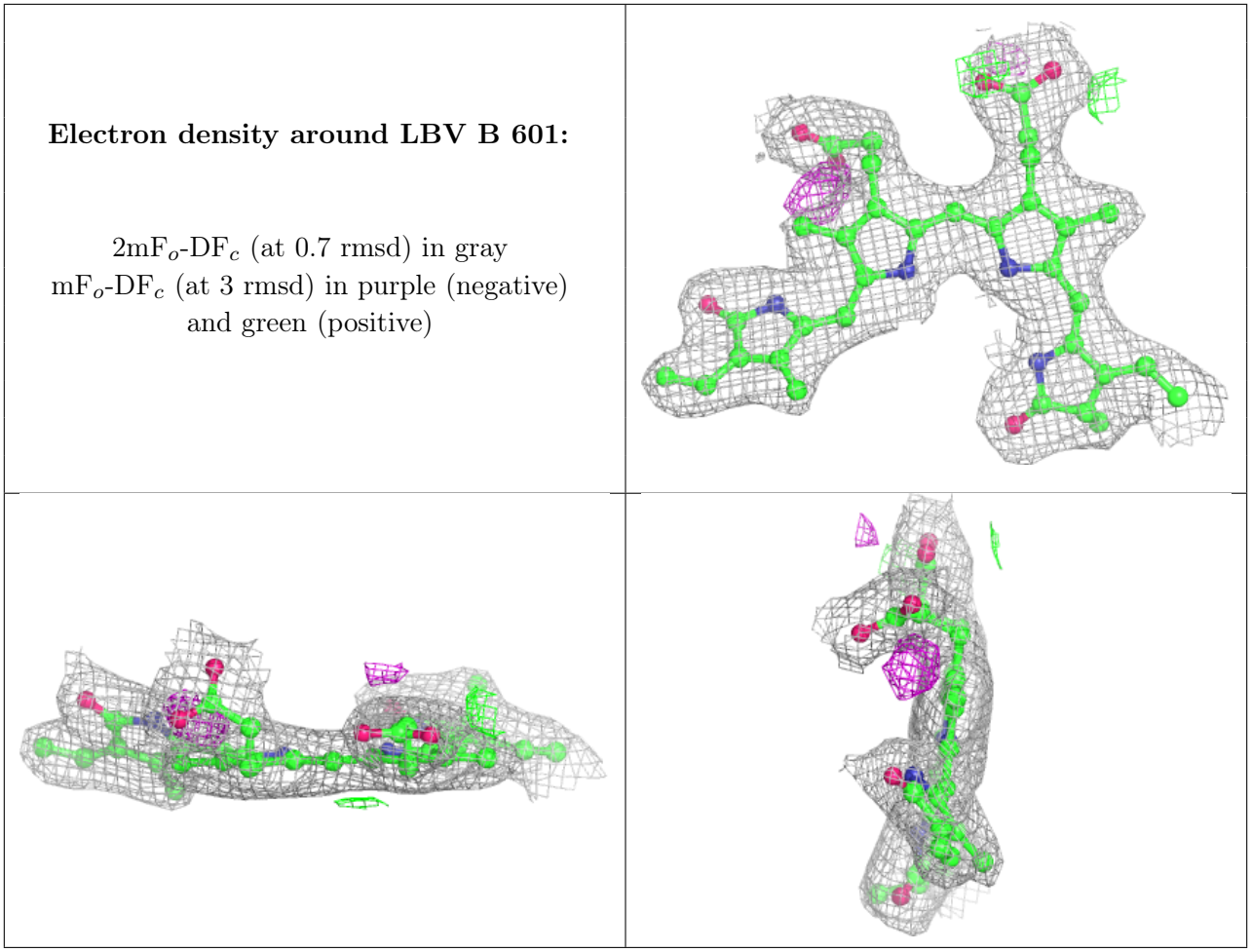
Electron density around LBV A 601:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



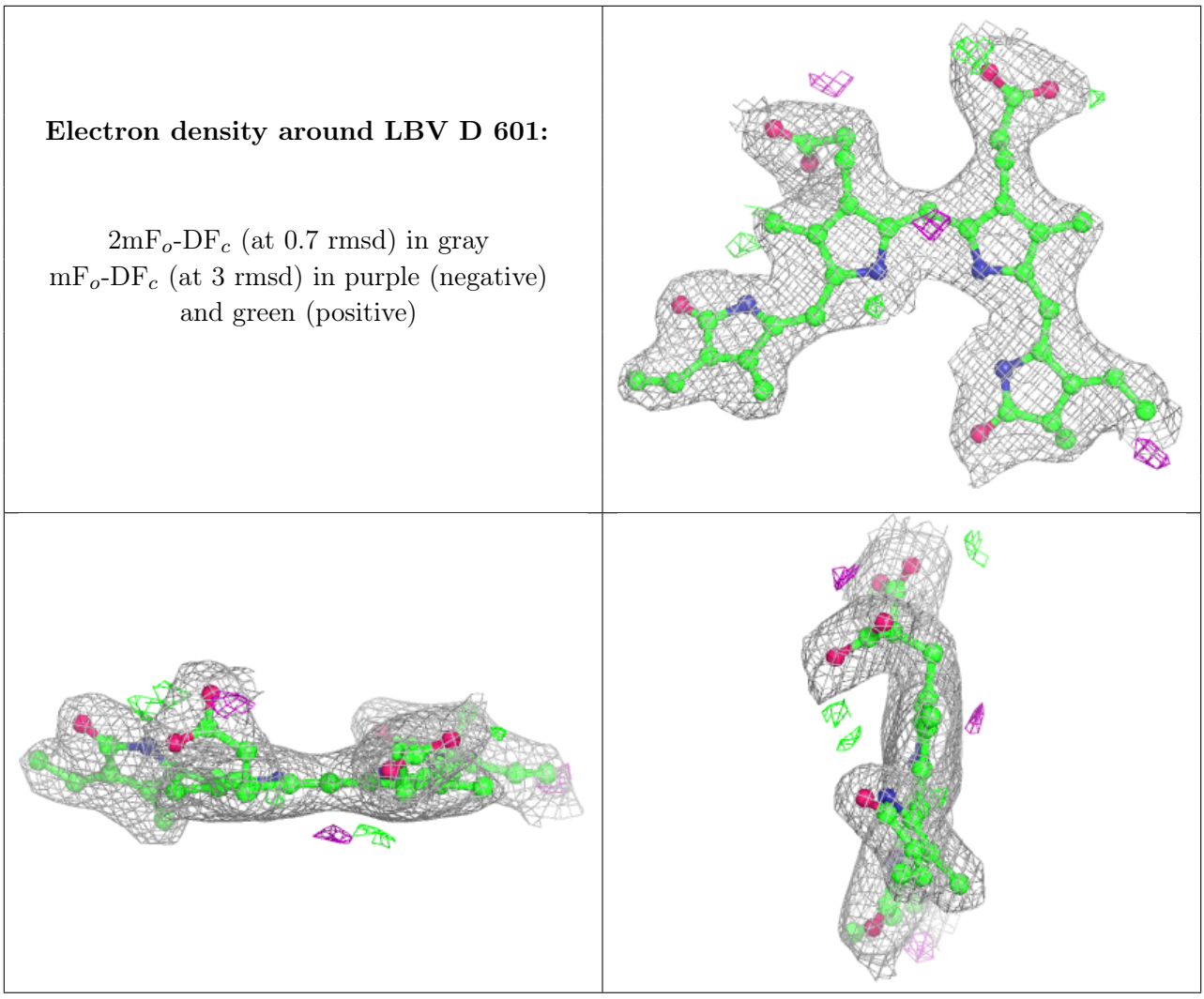
Electron density around LBV B 601:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around LBV D 601:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.